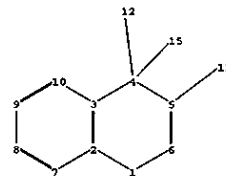
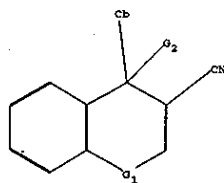


C:\stnweb\queries\100.str



chain nodes :

12 13 15

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

4-12 4-15 5-13

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10

exact/norm bonds :

1-2 1-6 3-4 4-5 4-12 4-15 5-6 5-13

normalized bonds :

2-3 2-7 3-10 7-8 8-9 9-10

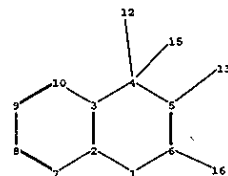
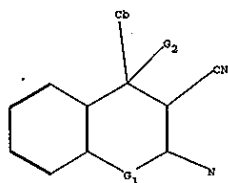
G1:O,S

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:Atom
13:CLASS 15:CLASS

C:\stnweb\Queries\100a.str



chain nodes :

12 13 15 16

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

4-12 4-15 5-13 6-16

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10

exact/norm bonds :

1-2 1-6 3-4 4-5 4-12 4-15 5-6 5-13 6-16

normalized bonds :

2-3 2-7 3-10 7-8 8-9 9-10

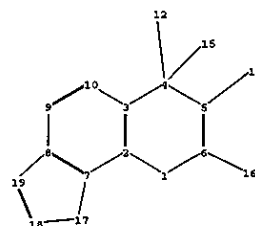
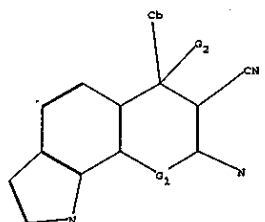
G1:O,S

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:Atom
13:CLASS 15:CLASS 16:CLASS

C:\stnweb\queries\100c.str



```

chain nodes :
  12 13 15 16
ring nodes :
  1 2 3 4 5 6 7 8 9 10 17 18 19
chain bonds :
  4-12 4-15 5-13 6-16
ring bonds :
  1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 7-17 8-9 8-19 9-10 17-18 18-19
exact/norm bonds :
  1-2 1-6 3-4 4-5 4-12 4-15 5-6 5-13 6-16 7-17 8-19 17-18 18-19
normalized bonds :
  2-3 2-7 3-10 7-8 8-9 9-10
isolated ring systems :
  containing 1 :

```

G1:O,S

G2:H,Ak

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:Atom
13:CLASS 15:CLASS 16:CLASS 17:Atom 18:Atom 19:Atom

```

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 SEP 09 CA/CAPLUS records now contain indexing from 1907 to the present
NEWS 4 AUG 05 New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS 5 AUG 13 Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 6 AUG 18 Data available for download as a PDF in RDISCLOSURE
NEWS 7 AUG 18 Simultaneous left and right truncation added to PASCAL
NEWS 8 AUG 18 FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation
NEWS 9 AUG 18 Simultaneous left and right truncation added to ANABSTR
NEWS 10 SEP 22 DIPPR file reloaded
NEWS 11 DEC 08 INPADOC: Legal Status data reloaded
NEWS 12 SEP 29 DISSABS now available on STN
NEWS 13 OCT 10 PCTFULL: Two new display fields added
NEWS 14 OCT 21 BIOSIS file reloaded and enhanced
NEWS 15 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 16 NOV 24 MSDS-CCOHS file reloaded
NEWS 17 DEC 08 CABA reloaded with left truncation
NEWS 18 DEC 08 IMS file names changed
NEWS 19 DEC 09 Experimental property data collected by CAS now available in REGISTRY
NEWS 20 DEC 09 STN Entry Date available for display in REGISTRY and CA/CAPLUS

NEWS EXPRESS NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01c, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:01:27 ON 12 DEC 2003

=> filereg

FILEREG IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 11:01:37 ON 12 DEC 2003
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 11 DEC 2003 HIGHEST RN 625827-33-0
 DICTIONARY FILE UPDATES: 11 DEC 2003 HIGHEST RN 625827-33-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d 11

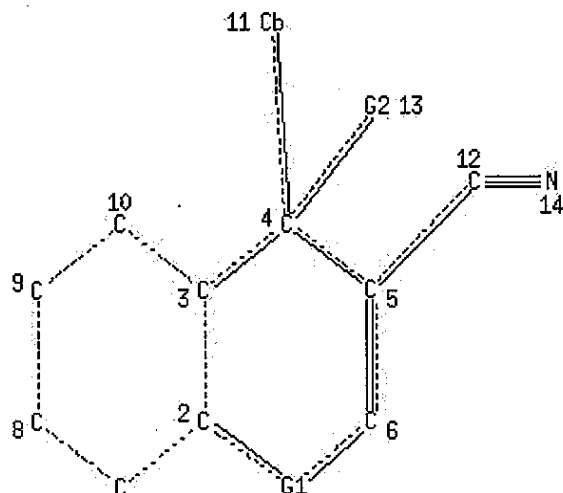
L1 HAS NO ANSWERS

L1 STR

H 17 Ak 18

0 15 S 16

Page 1-A



Page 1-B

7

1

Page 2-B

VAR G1=15/16

VAR G2=17/18

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3

NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS R AT 10
NSPEC IS C AT 11
NSPEC IS C AT 12
NSPEC IS C AT 13
NSPEC IS C AT 14
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 12 14 17 18
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

=> s 11

SAMPLE SEARCH INITIATED 11:06:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 574 TO ITERATE

100.0% PROCESSED 574 ITERATIONS
SEARCH TIME: 00.00.01

49 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 10043 TO 12917
PROJECTED ANSWERS: 560 TO 1400

L2 49 SEA SSS SAM L1

=>

L3 STRUCTURE UPLOADED

=> d 13

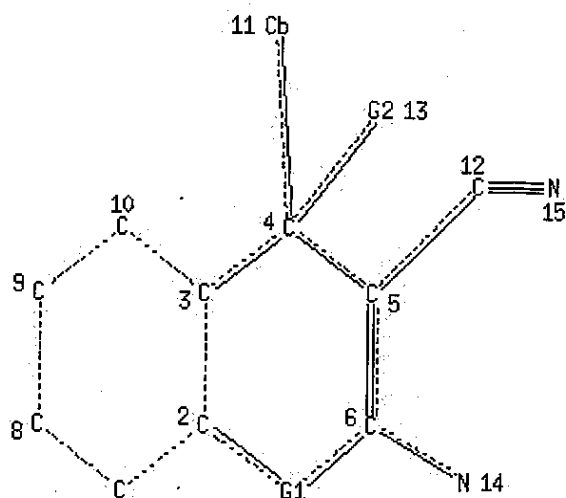
L3 HAS NO ANSWERS

L3 STR

H 18 AK 19

0 16 S 17

Page 1-A



Page 1-B

7 1

Page 2-B

VAR G1=16/17

VAR G2=18/19

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15

DEFAULT MLEVEL IS ATOM

MLEVEL	IS	CLASS	AT	12	14	15	18	19
--------	----	-------	----	----	----	----	----	----

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

=> s 13

SAMPLE SEARCH INITIATED 11:07:36 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 298 TO ITERATE

```
100.0% PROCESSED      298 ITERATIONS
SEARCH TIME: 00.00.01
```

49 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS:	4925 TO	6995
PROJECTED ANSWERS:	560 TO	1400

L4 49 SEA SSS SAM L3

=>

L5 STRUCTURE UPLOADED

=> d 15

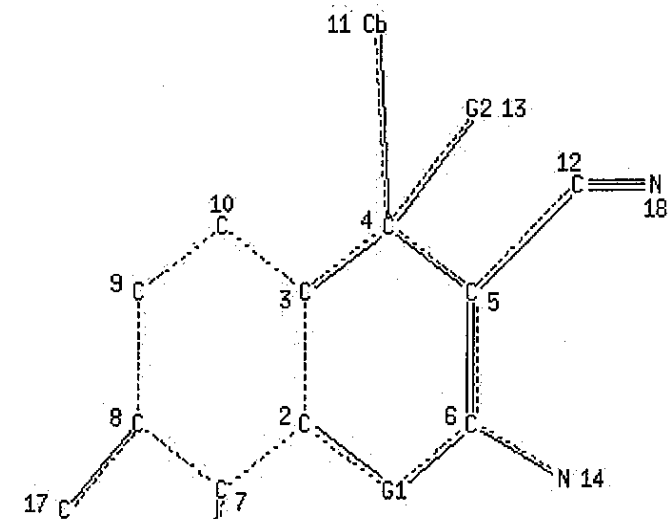
L5 HAS NO ANSWERS

L5 STR

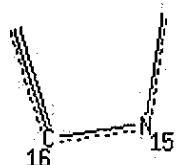
H 21 Ak 22

0 19 S 20

Page 1-A



Page 1-B



Page 2-B

VAR G1=19/20

VAR G2=21/22

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS R	AT	15
NSPEC	IS R	AT	16
NSPEC	IS R	AT	17

NSPEC IS C AT 18
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 12 14 18 21 22
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC I
 NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

=> s 15
 SAMPLE SEARCH INITIATED 11:08:27 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 4 TO ITERATE

100.0% PROCESSED 4 ITERATIONS 0 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 4 TO 200
 PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 full
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 11:08:31 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 115 TO ITERATE

100.0% PROCESSED 115 ITERATIONS 10 ANSWERS
 SEARCH TIME: 00.00.01

L7 10 SEA SSS FUL L5

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	152.55	152.76

FILE 'HCAPLUS' ENTERED AT 11:08:36 ON 12 DEC 2003
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FILE COVERS 1907 - 12 Dec 2003 VOL 139 ISS 25
 FILE LAST UPDATED: 11 Dec 2003 (20031211/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 17

L8 1 L7

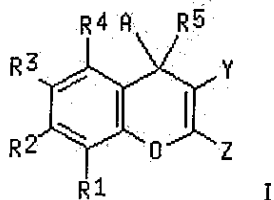
=> d 18, ibib abs fhitr, 1

L8 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Citing
Text References

ACCESSION NUMBER: 2002:888735 HCAPLUS
DOCUMENT NUMBER: 137:369971
TITLE: Preparation of substituted 4H-chromenes and analogs as activators of caspases and inducers of apoptosis and their uses against cancer and other disorders
INVENTOR(S): Cai, Sui Xiong; Zhang, Hong; Jiang, Songchun; Storer, Richard
PATENT ASSIGNEE(S): Cytovia, Inc., USA
SOURCE: PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002092594	A1	20021121	WO 2002-US15399	20020516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003065018	A1	20030403	US 2002-146138	20020516
<u>PRIORITY APPLN. INFO.:</u>			<u>US 2001-290997P</u>	P 20010516
OTHER SOURCE(S):		MARPAT 137:369971		
GI				



AB The present invention is directed to substituted 4H-chromenes and analogs thereof (shown as I; e.g. 2-amino-3-cyano-7-hydroxy-4-(3-bromo-4,5-dimethoxyphenyl)-4H-chromene). It also relates to the discovery that I are activators of caspases and inducers of apoptosis and, therefore, can be used to induce cell death in a variety of clin. conditions in which controlled growth and spread of abnormal cells occurs. In I: R1-R4 = H,

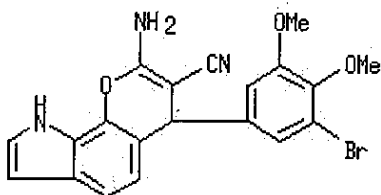
halo, haloalkyl, aryl, fused aryl, carbocyclic, heterocyclic, heteroaryl, C1-10 alkyl, alkenyl, alkynyl, arylalkyl, arylalkenyl, arylalkynyl, heteroarylalkyl, heteroarylalkenyl, heteroarylalkynyl, carbocycloalkyl, heterocycloalkyl, hydroxyalkyl, aminoalkyl, carboxyalkyl, nitro, amino, cyano, acylamido, hydroxy, thiol, acyloxy, azido, alkoxy, carboxy, methylenedioxy, carbonylamido or alkylthio; or R1 and R2, or R2 and R3, or R3 and R4, taken together with the atoms to which they are attached form an aryl, heteroaryl, partially satd. carbocyclic or partially satd. heterocyclic group, wherein said group is optionally substituted. R5 is H or C1-10 alkyl; A is optionally substituted and is aryl, heteroaryl, satd. carbocyclic, partially satd. carbocyclic, satd. heterocyclic, partially satd. heterocyclic or arylalkyl; Y is CN, COR7, CO2R7 or CONRxRy, wherein R7, Rx and Ry = H, C1-10 alkyl, haloalkyl, aryl, fused aryl, carbocyclic, heterocyclic, heteroaryl, alkenyl, alkynyl, arylalkyl, arylalkenyl, arylalkynyl, heteroarylalkyl, heteroarylalkenyl, heteroarylalkynyl, carbocycloalkyl, heterocycloalkyl, hydroxyalkyl or aminoalkyl; or Rx and Ry are taken together with the N to which they are attached to form a heterocycle; and Z is NR8R9, NHCOR8, N(COR9)2, N(COR8)(COR9), N:CHOR8 or N:CHR8, wherein R8 and R9 = H, C1-4 alkyl or aryl, or R8 and R9 are combined together with the group attached to them to form a heterocycle. The EC50 values for >80 I against T-47D and ZR-75-1 human breast cancer cell lines are tabulated, e.g. 30 and 25 nM, resp., for 2-amino-3-cyano-4-(3-bromo-4,5-dimethoxyphenyl)-4H-indolo[7,6-b]pyran. Although the methods of prepn. are not claimed, 81 example preps. are included.

IT 475576-80-8P, 2-Amino-3-cyano-4-(3-bromo-4,5-dimethoxyphenyl)-4H-indolo[7,6-b]pyran

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; prepn. of substituted 4H-chromenes and analogs as activators of caspases and inducers of apoptosis and their uses against cancer and other disorders)

RN 475576-80-8 HCAPLUS

CN Pyrano[3,2-g]indole-3-carbonitrile, 2-amino-4-(3-bromo-4,5-dimethoxyphenyl)-4,9-dihydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
6.79	159.55

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-0.65	-0.65

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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 11:01:27 ON 12 DEC 2003)

FILE 'REGISTRY' ENTERED AT 11:01:37 ON 12 DEC 2003

```
L1          STRUCTURE UPLOADED
L2          49 S L1
L3          STRUCTURE UPLOADED
L4          49 S L3
L5          STRUCTURE UPLOADED
L6          0 S L5
L7          10 S L5 FULL
```

FILE 'HCAPLUS' ENTERED AT 11:08:36 ON 12 DEC 2003

```
L8          1 S L7
```

FILE 'CAOLD' ENTERED AT 11:08:48 ON 12 DEC 2003

=> s 17

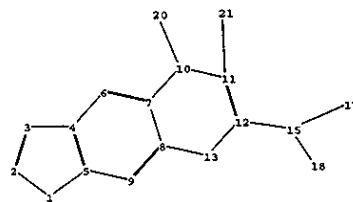
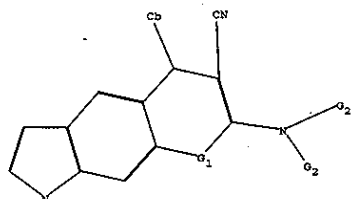
```
L9          0 L7
```

=> log y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.40	159.95
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.65

STN INTERNATIONAL LOGOFF AT 11:08:56 ON 12 DEC 2003

C:\stnweb\Queries\9.str



chain nodes :

15 17 18 20 21

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

10-20 11-21 12-15 15-17 15-18

ring bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 7-10 8-9 8-13 10-11 11-12 12-13

exact/norm bonds :

1-2 1-5 2-3 3-4 7-10 8-13 10-11 10-20 11-12 11-21 12-13 12-15 15-17 15-18

normalized bonds :

4-5 4-6 5-9 6-7 7-8 8-9

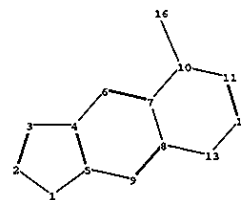
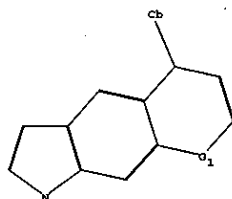
G1:O,S

G2:Ak,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 15:CLASS 17:CLASS 18:CLASS 20:Atom 21:CLASS

C:\stnweb\Queries\9a.str



chain nodes :

16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

10-16

ring bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 7-10 8-9 8-13 10-11 11-12 12-13

exact/norm bonds :

1-2 1-5 2-3 3-4 7-10 8-13 10-11 10-16 11-12 12-13

normalized bonds :

4-5 4-6 5-9 6-7 7-8 8-9

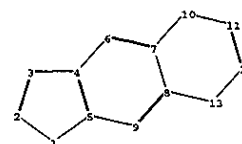
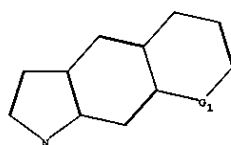
G1:O,S

G2:Ak,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 16:Atom

C:\stnweb\Queries\9b.str



ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

ring bonds :

1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 7-10 8-9 8-13 10-11 11-12 12-13

exact/norm bonds :

1-2 1-5 2-3 3-4 7-10 8-13 10-11 11-12 12-13

normalized bonds :

4-5 4-6 5-9 6-7 7-8 8-9

G1:O,S

G2:Ak,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom

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NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 SEP 09 CA/CAPLUS records now contain indexing from 1907 to the present
NEWS 4 AUG 05 New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS 5 AUG 13 Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 6 AUG 18 Data available for download as a PDF in RDISCLOSURE
NEWS 7 AUG 18 Simultaneous left and right truncation added to PASCAL
NEWS 8 AUG 18 FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation
NEWS 9 AUG 18 Simultaneous left and right truncation added to ANABSTR
NEWS 10 SEP 22 DIPPR file reloaded
NEWS 11 DEC 08 INPADOC: Legal Status data reloaded
NEWS 12 SEP 29 DISSABS now available on STN
NEWS 13 OCT 10 PCTFULL: Two new display fields added
NEWS 14 OCT 21 BIOSIS file reloaded and enhanced
NEWS 15 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 16 NOV 24 MSDS-CCOHS file reloaded
NEWS 17 DEC 08 CABA reloaded with left truncation
NEWS 18 DEC 08 IMS file names changed
NEWS 19 DEC 09 Experimental property data collected by CAS now available in REGISTRY
NEWS 20 DEC 09 STN Entry Date available for display in REGISTRY and CA/CAPLUS

NEWS EXPRESS NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01c, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:28:25 ON 12 DEC 2003

=> g

G IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

For a list of commands available to you in the current file, enter

"HELP COMMANDS" at an arrow prompt (=>).

=> file reg

COST IN U.S. DOLLARS

SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST

0.21 0.21

FILE 'REGISTRY' ENTERED AT 10:28:33 ON 12 DEC 2003
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 11 DEC 2003 HIGHEST RN 625827-33-0
 DICTIONARY FILE UPDATES: 11 DEC 2003 HIGHEST RN 625827-33-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
 information enter HELP PROP at an arrow prompt in the file or refer
 to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> d 11

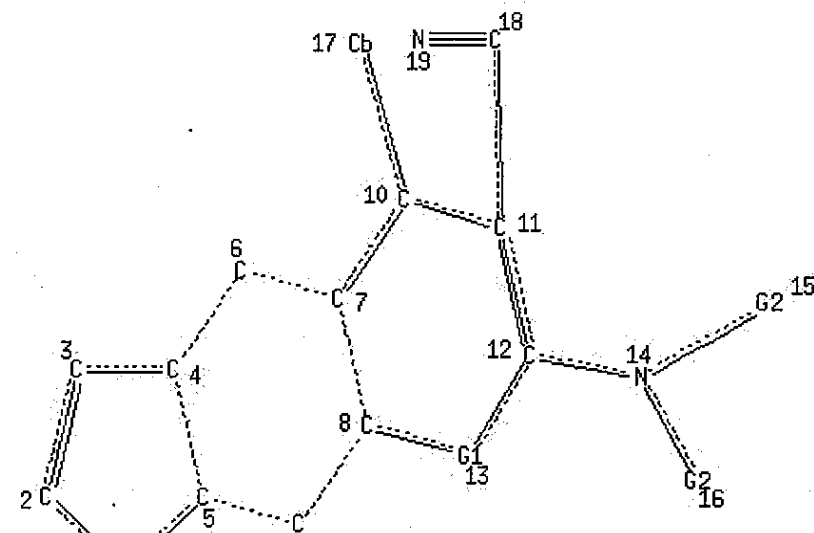
L1 HAS NO ANSWERS

L1 STR

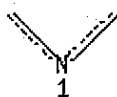
AK 22H 23

0 20 5 21

Page 1-A



Page 1-B



Page 2-B

VAR G1=20/21

VAR G2=22/23

NODE ATTRIBUTES:

```

NSPEC   IS R      AT   1
NSPEC   IS R      AT   2
NSPEC   IS R      AT   3
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS R      AT   7
NSPEC   IS R      AT   8
NSPEC   IS R      AT   9
NSPEC   IS R      AT  10
NSPEC   IS R      AT  11
NSPEC   IS R      AT  12
NSPEC   IS R      AT  13
NSPEC   IS C      AT  14
NSPEC   IS C      AT  15
NSPEC   IS C      AT  16
NSPEC   IS C      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS AT  14 18 19 22 23
DEFAULT ECLEVEL IS LIMITED

```

GRAPH ATTRIBUTES:

```

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  23

```

```

STEREO ATTRIBUTES: NONE

```

```

=> s 11

```

```

SAMPLE SEARCH INITIATED 10:31:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      42 TO ITERATE

```

```

100.0% PROCESSED      42 ITERATIONS      0 ANSWERS
SEARCH TIME: 00.00.01

```

```

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   452 TO      1228
PROJECTED ANSWERS:      0 TO        0

```

```

L2          0 SEA SSS SAM L1

```

```

=> s 11 full

```

```

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 10:31:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      997 TO ITERATE

```

```

100.0% PROCESSED      997 ITERATIONS      0 ANSWERS
SEARCH TIME: 00.00.01

```

```

L3          0 SEA SSS FUL L1

```

```

=>

```

```

L4          STRUCTURE UPLOADED

```

```

=> d 14

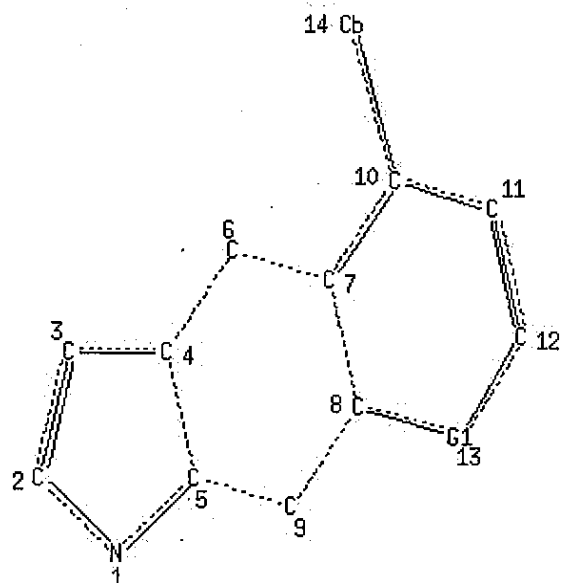
```

L4 HAS NO ANSWERS

L4 STR

0 15 S 16

Page 1-A



Page 1-B

VAR G1=15/16

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13
NSPEC	IS C	AT	14

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

=> s 14

SAMPLE SEARCH INITIATED 10:32:06 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 3002 TO ITERATE

33.3% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**
 PROJECTED ITERATIONS: 56755 TO 63325
 PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s 14 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 10:32:10 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 59948 TO ITERATE

100.0% PROCESSED 59948 ITERATIONS
 SEARCH TIME: 00.00.01

0 ANSWERS

L6 0 SEA SSS FUL L4

=>

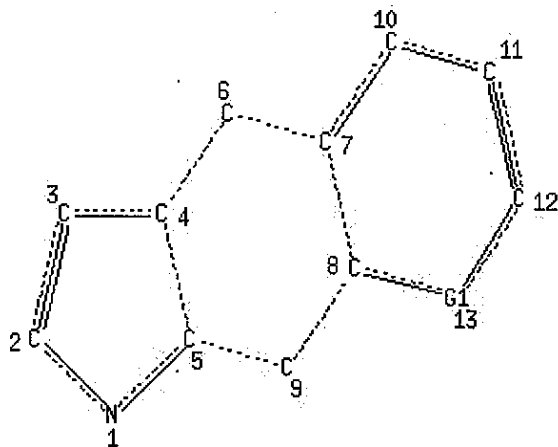
L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR

0 14 S 15
 Page 1-A



Page 1-B

VAR G1=14/15

NODE ATTRIBUTES:

NSPEC	IS R	AT	1
NSPEC	IS R	AT	2
NSPEC	IS R	AT	3
NSPEC	IS R	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS R	AT	11
NSPEC	IS R	AT	12
NSPEC	IS R	AT	13

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

=> s 17

SAMPLE SEARCH INITIATED 10:32:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3002 TO ITERATE

33.3% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 56755 TO 63325
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 10:32:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 59948 TO ITERATE

100.0% PROCESSED 59948 ITERATIONS 24 ANSWERS
SEARCH TIME: 00.00.01

L9 24 SEA SSS FUL L7

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	446.05	446.26

FILE 'HCAPLUS' ENTERED AT 10:33:01 ON 12 DEC 2003

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FILE COVERS 1907 - 12 Dec 2003 VOL 139 ISS 25
FILE LAST UPDATED: 11 Dec 2003 (20031211/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 19

L10 8 L9

=> d 110, ibib abs fhitr, 1-8

L10 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

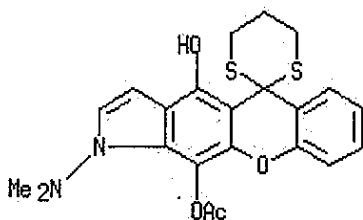
Full Text	Citing References
-----------	-------------------

ACCESSION NUMBER: 1996:689416 HCAPLUS
 DOCUMENT NUMBER: 126:7949
 TITLE: Novel Construction of Highly-Substituted Xanthenes
 AUTHOR(S): Sun, Lijun; Liebeskind, Lanny S.
 CORPORATE SOURCE: Sanford S. Atwood Chemistry Center, Emory University, Atlanta, GA, 30322, USA
 SOURCE: Journal of the American Chemical Society (1996), 118(49), 12473-12474
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 126:7949

AB O-, C-Dianions generated from dithiane protected salicylaldehydes condense with esters of squaric acid in a two-step process to provide γ -benzopyrone-fused cyclobutenediones, with the benzopyrone still protected as the dithiane. These versatile cyclobutenediones undergo regiospecific 1,2-addn. of unsatd. organolithium reagents (Ph, substituted Ph, 1- and 2-naphthyl, 2- and 3-furyl, 2-thienyl, 2-pyrrolyl, 2-indolyl, β -styryl, 2-dihydropyranyl) at the most electrophilic and least hindered cyclobutenedione carbonyl group. The 1,2-adducts rearrange either spontaneously at room temp. or on brief warming in THF soln. to give, after hydrolysis of the dithiane, a wide variety of substituted xanthenes and xanthenes linearly fused to arom., heteroarom., and heterocyclic rings.

IT **184023-43-6P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of xanthenes)

RN **184023-43-6** HCAPLUS
 CN Spiro[[1]benzopyrano[3,2-f]indole-5(1H),2'-[1,3]dithiane]-4,11-diol, 1-(dimethylamino)-, 11-acetate (9CI) (CA INDEX NAME)

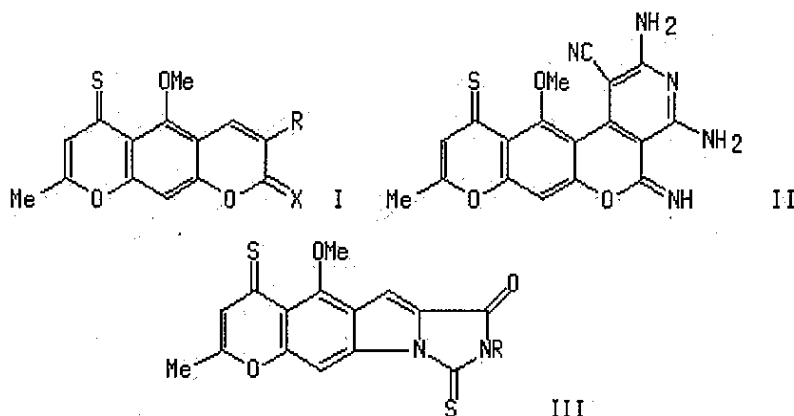


L10 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
-----------	-------------------

ACCESSION NUMBER: 1991:101768 HCAPLUS
 DOCUMENT NUMBER: 114:101768
 TITLE: Benzodipyranthione derivatives of expected biological activities
 AUTHOR(S): Abdelaziz, Mahfouz A.

CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
 SOURCE: Egyptian Journal of Pharmaceutical Sciences (1990),
 31(1-4), 561-70
 CODEN: EJPSBZ; ISSN: 0301-5068
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



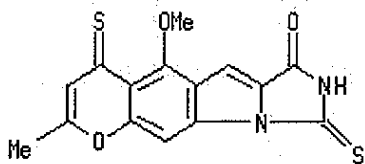
AB 6-Formyl-7-hydroxy-5-methoxy-2-methylbenzopyran-4-thione reacted with cyanoethanoic acid hydrazide, 2-amino-1,1,3-tricyanoprop-1-ene, benzoylacetonitrile, malononitrile and 2-thiohydantoin to afford heterocycles, e.g., benzodipyrans I [X=O,NH; R = CONHNH₂; X=NH, R = C(NH₂):C(CN)₂; X = O, NH; R = C(Ph), cyano], pyranobenzopyranopyridine II and benzopyranopyrroloimidazolinethiones III (R = H, Ph).

IT 132369-76-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 132369-76-7 HCAPLUS

CN 4H,7H-Imidazo[1,5-a]pyrano[3,2-f]indol-7-one, 8,9-dihydro-5-methoxy-2-methyl-4,9-dithioxo- (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 1990:7422 HCAPLUS

DOCUMENT NUMBER: 112:7422

TITLE: New synthesis of chromonopyrroloimidazolinones and arylidenethioxoimidazolinones. Study of their antimicrobial activities

AUTHOR(S): Aziz, Mahfouz A. Abdel; Riad, Bahia Y.; Shalaby, A. M.

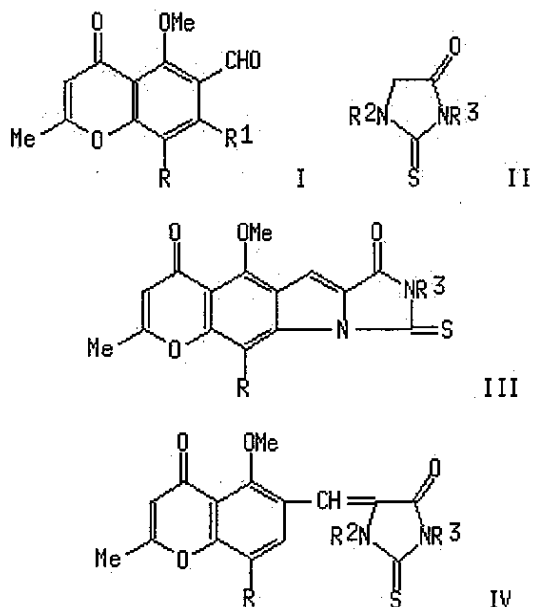
CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt

SOURCE: Archives of Pharmacal Research (1989), 12(1), 12-16

CODEN: APHRDQ; ISSN: 0253-6269

DOCUMENT TYPE: Journal

LANGUAGE: English
GI



AB 6-Formyl-5-methoxy-2-methylchromone derivs. I ($R = H, NO_2, Br, R_1 = OH; R = H, R_1 = OMe$) condensed with 2-thioxo-4-imidazolinones II ($R_2 = H, R_3 = H, Ph; R_2 = Ph, R_3 = H$) to form the corresponding chromonopyrroloimidazolinones III or the arylidenethioxoimidazolinones IV. The activity of the imidazole moiety NH of III ($R = R_3 = H$) (V) was confirmed by formation of the Mannich bases. Moreover, alkylation of V was gave alkylmercapto derivs. The antimicrobial activities of compds. II and IV were studied.

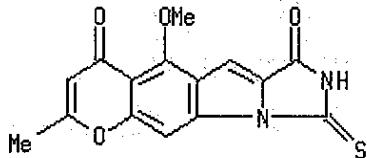
IT 124041-37-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and alkylation or Mannich reactions of)

RN 124041-37-8 HCAPLUS

CN 4H,7H-Imidazo[1,5-a]pyrano[3,2-f]indole-4,7-dione, 8,9-dihydro-5-methoxy-2-methyl-9-thioxo- (9CI) (CA INDEX NAME)



L10 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full
Text

Citing
References

ACCESSION NUMBER: 1989:457344 HCAPLUS

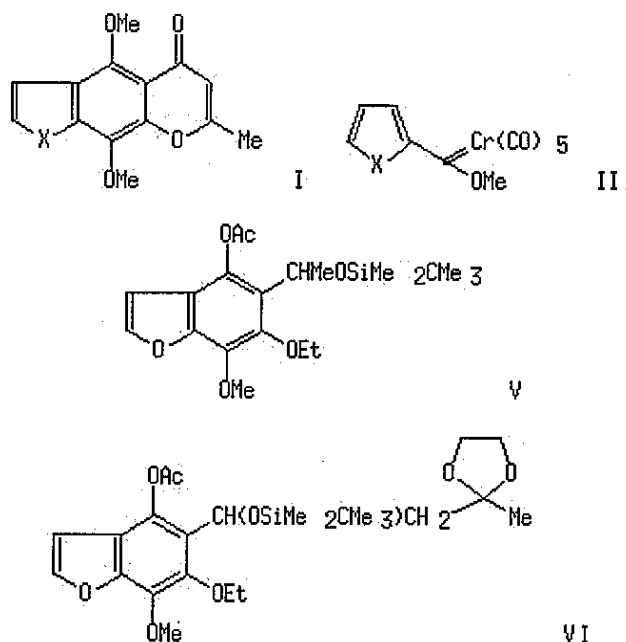
DOCUMENT NUMBER: 111:57344

TITLE: Synthesis of khellin and its analogs via chromium carbene complexes

AUTHOR(S): Yamashita, A.; Toy, A.; Scahill, T. A.

CORPORATE SOURCE: Res. Lab., Upjohn Co., Kalamazoo, MI, 49001, USA

SOURCE: Journal of Organic Chemistry (1989), 54(15), 3625-34
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 111:57344
 GI

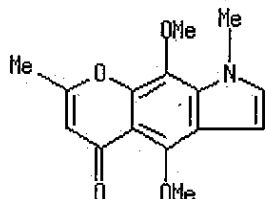


AB The synthesis of khellin (I; X = O), a lipid-altering and antiatherosclerotic furochromone, was accomplished by two different routes in six and seven steps, resp. The key steps in two alternative approaches are the cycloaddn. reactions of a furan-methoxy chromium carbene complex II (X = O) with EtOC≡CCHROSiMe₂CMe₃ [R = Me (III), 2-methyl-1,3-dioxolan-2-yl (IV)] to provide the direct construction of the benzofuran acetates V and VI, which bear the functional groups necessary for formation of the γ-pyrone ring. The reactions of II (X = O) with alkoxyalkynes in the presence of Ac₂O and Et₃N in THF provided the acetate derivs. of the desired benzofurans in fair to good yields. The alkoxyalkyne III introduces the acetyl group precursor and IV bears the masked β-diketone unit. The benzofuran acetate V leads to khellinone in four steps by direct conversion of the acetate to a Me ether, the conversion of the silyloxy to the ketone, and the selective cleavage of the Et ether. The other benzofuran acetate VI leads to khellinquione in five steps by the direct conversion of the acetate to the Me ether, the conversion of the silyloxy ether to a ketone, oxidn. of the p-dimethoxybenzene ring, and sequential aq. acid-catalyzed pyrone ring formation. Khellinone and khellinquione are converted to I independently by known procedures. These two synthetic routes are applied to the syntheses of khellin analogs, such as the pyrrole (I; X = NMe) and phenyl (I; X = CH:CH) analogs of khellin, using the reactions of the resp. pyrrolyl or Ph chromium carbene complexes II (X = NMe, CH:CH) with III and IV.

IT 121444-68-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (total synthesis of)

RN 121444-68-6 HCAPLUS
 CN Pyrano[3,2-f]indol-4(8H)-one, 5,9-dimethoxy-2,8-dimethyl- (9CI) (CA INDEX NAME)



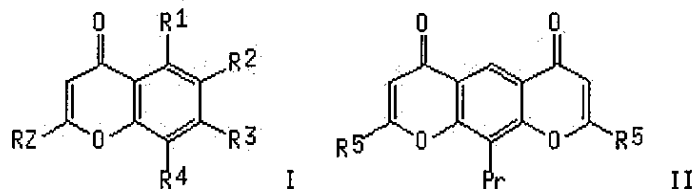
Z = Me

L10 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text Citing
 References

ACCESSION NUMBER: 1986:68836 HCAPLUS
 DOCUMENT NUMBER: 104:68836
 TITLE: Benzopyran derivatives and anti-asthma compositions containing them
 INVENTOR(S): Gould, Kenneth John; Suschitzky, John Louis; Dicker, Ian Douglas
 PATENT ASSIGNEE(S): Fisons PLC, UK
 SOURCE: Eur. Pat. Appl., 118 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 150966	A2	19850807	EP 1985-300381	19850121
EP 150966	A3	19860625		
EP 150966	B1	19890712		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 44530	E	19890715	AT 1985-300381	19850121
ZA 8500550	A	19851127	ZA 1985-550	19850123
DK 8500313	A	19850727	DK 1985-313	19850124
DK 162893	B	19911223		
FI 8500324	A	19850727	FI 1985-324	19850125
FI 84482	B	19910830		
FI 84482	C	19911210		
NO 8500303	A	19850729	NO 1985-303	19850125
JP 60163877	A2	19850826	JP 1985-11134	19850125
ES 539846	A1	19870501	ES 1985-539846	19850125
CA 1268460	A1	19900501	CA 1985-472848	19850125
IL 74166	A1	19901105	IL 1985-74166	19850125
US 4670452	A	19870602	US 1985-695459	19850128
US 4698345	A	19871006	US 1985-695460	19850128
AU 8538194	A1	19850801	AU 1985-38194	19850130
AU 582135	B2	19890316		
CA 1250584	A1	19890228	CA 1985-473177	19850130
CN 85105645	A	19870128	CN 1985-105645	19850724
CN 1010855	B	19901219		
ES 554962	A1	19870701	ES 1986-554962	19860514
PRIORITY APPLN. INFO.:			GB 1984-2047	19840126
			GB 1984-2577	19840201
			EP 1985-300381	19850121



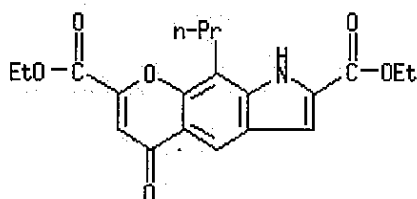
AB Antiasthmatic (no data) title compds. [I; R = CO₂H, tetrazol-5-yl; adjacent pairs of R₁-R₄ = atoms required to complete an (un)substituted 5- or 6-membered arom. or heteroarom. ring; Z = bond, (CH₂)_m, arylene, m = 1-10] were prepd. Thus, di-Et 4,6-dioxo-10-propyl-4H,6H-benzo[1,2-b:5,4-b']dipyran-2,8-dicarboxylate (II, R₅ = CO₂Et) was treated with NH₃ in EtOH to give II (R₅ = CONH₂) which was dehydrated by heating in DMF with POCl₃ to give II (R₅ = cyano). This was heated at 60° with NaN₃ in DMF to give II (R₅ = 1H-tetrazol-5-yl), converted to its di-Na salt.

IT 99370-80-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sapon. of)

RN 99370-80-6 HCAPLUS

CN Pyrano[3,2-f]indole-2,7-dicarboxylic acid, 4,8-dihydro-4-oxo-9-propyl-, diethyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Citing
Text References

ACCESSION NUMBER: 1972:434319 HCAPLUS
DOCUMENT NUMBER: 77:34319
TITLE: Antiinflammatory 2,3-bis(p-methoxyphenyl)indole-5-carboxylic acid derivatives
INVENTOR(S): Szmuszkowicz, Jacob
PATENT ASSIGNEE(S): Upjohn Co.
SOURCE: U.S., 8 pp. Division of U.S. 3,565,912 (CA 75:35734t).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3654308	A	19720404	US 1970-65315	19700819
PRIORITY APPLN. INFO.:			US 1970-65315	19700819

GI For diagram(s), see printed CA Issue.

AB Division of U.S. 3,565,912 (CA 75: 35734t). Four antiinflammatory 5-alkanoyl-2,3-bis(p-methoxyphenyl)indoles I (R = H, Me; R₁ = H, Me, Ac)

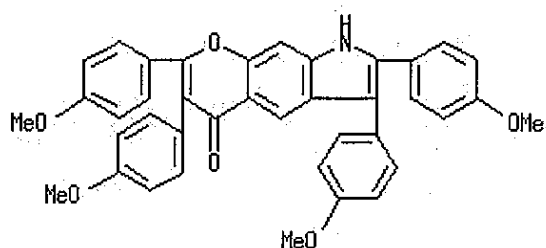
were prepd. Anisoin and p-H₂NC₆H₄CO₂Et refluxed 2 hr in xylene in the presence of p-MeC₆H₄SO₃H gave 81% Et p-[[p-methoxy- α -(p-methoxyphenyl)phenacyl]amino]benzoate, which on further heating with p-H₂NC₆H₄CO₂Et and pMeC₆H₄SO₃H gave II (R = Et, R₁ = H). Refluxing II (R = Et, R₁ = H) in aq. alc. with KOH gave its corresponding acid, which was then refluxed in C₆H₆ with SOCl₂, and the product added to CdCl₂ and MeMgBr in Et₂O, refluxed 4 hr to give I (R = Me, R₁ = H). Formulations of I were given. The following II (R₁ = H) (R = (CH₂)₂OH, Et, H) were claimed.

IT **23659-79-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN **23659-79-2** HCAPLUS

CN **Pyrano[3,2-f]indol-4(8H)-one, 2,3,6,7-tetrakis(4-methoxyphenyl)- (9CI)**
(CA INDEX NAME)



L10 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

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Text References

ACCESSION NUMBER: 1971:435734 HCAPLUS
DOCUMENT NUMBER: 75:35734
TITLE: Antiinflammatory 5-alkanoyl-2,3-bis(p-methoxyphenyl)indoles
INVENTOR(S): Szmuszkovicz, Jacob
PATENT ASSIGNEE(S): Upjohn Co.
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3565912	A	19710223	US 1969-794402	19690127
PRIORITY APPLN. INFO.:			US 1969-794402	19690127

GI For diagram(s), see printed CA Issue.

AB The title indoles (I, R = H, Me, or Ac; R₁ = H, Me, Et, HO, EtO, iso-Pr) are produced by heating p-H₂NC₆H₄CO₂R₁ with anisoin in the presence of an acid catalyst and further heating with an alkyl p-aminobenzoate and acid catalyst, saponifying the alkyl 2,3-bis(p-methoxyphenyl)indole-5-carboxylate, converting to the acyl chloride and treating the chloride in the presence of CdCl₂ with RMgX. The product was treated with NaH and alkyl halide or acyl halide. Alternatively, p-H₂NNHC₆H₄CO₂R₁ was heated with deoxyanisoin, the mixt. refluxed with alc. HCl or HOCH₂CH₂OH, and the ester of 2,3-bis(p-methoxyphenyl)-indole-5-carboxylic acid treated to give the free acid, which was then converted as above to I. Thus anisoin and p-H₂NC₆H₄CO₂Et refluxed in xylene in the presence of p-MeC₆H₄SO₃H yielded 81% Et p-[[p-methoxy α -(p-methoxyphenyl)phenacyl]-amino benzoate,

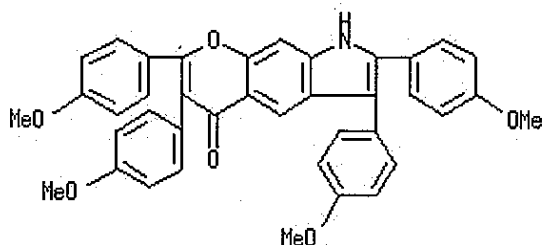
which was heated with p-H₂NC₆H₄CO₂Et to give I (R = H, R₁ = OEt) (II) Et 2,3-bis(p-methoxyphenyl)indole-5-carboxylate. II refluxed in aq. alc with KOH gave I (R = H, R₁ = OH) (III), m. 295-7°. Equimolar amts. of p-EtO₂CC₆H₄NHNH₂ and deoxyanisoin refluxed with HOCH₂CH₂OH yielded 2-(hydroxyethyl)-2,3-bis(p-methoxyphenyl)indole-5-carboxylate, which was hydrolyzed and acidified as above to give III. III refluxed in C₆H₆ with SOCl₂ and the product added to CdCl₂ and MeMgBr in Et₂O and refluxed 4 hr gave I (R = Me, R₁ = H) (IV), m. 227-3°.

IT 23659-79-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 23659-79-2 HCAPLUS

CN Pyrano[3,2-f]indol-4(8H)-one, 2,3,6,7-tetrakis(4-methoxyphenyl)- (9CI)
(CA INDEX NAME)



L10 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2003 ACS on STN

Full Text	Citing References
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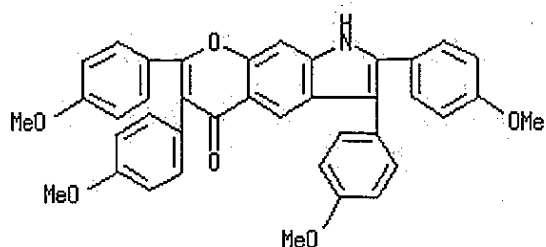
ACCESSION NUMBER:	1969:491199 HCAPLUS
DOCUMENT NUMBER:	71:91199
TITLE:	Synthesis and antiinflammatory activity of 5-substituted 2,3-bis(p-methoxyphenyl)indoles
AUTHOR(S):	Youngdale, Gilbert A.; Glenn, E. Myles; Lednicer, Daniel; Szmuszkowicz, Jacob
CORPORATE SOURCE:	Res. Lab., Upjohn Co., Kalamazoo, MI, USA
SOURCE:	Journal of Medicinal Chemistry (1969), 12, 948-9 CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE:	Journal
LANGUAGE:	English
GI	For diagram(s), see printed CA Issue.
AB	p-Carbethoxyphenylhydrazine is treated with deoxyanisoin to give Et 2,3-bis(p-carbethoxyphenyl)indole-5-carboxylate (I), 2,3,6,7-tetrakis(p-carbethoxyphenyl)pyrano-[3,2-f]indolin-4(8H)-one (II) is obtained as a by-product. I is transesterified to give III; IV and V are prepd. from III. The antiinflammatory activity of V is equal to that of VI.

IT 23659-79-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 23659-79-2 HCAPLUS

CN Pyrano[3,2-f]indol-4(8H)-one, 2,3,6,7-tetrakis(4-methoxyphenyl)- (9CI)
(CA INDEX NAME)



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